PROJECT NUMBER: 6502
PROJECT TITLE: Environmental Tobacco Smoke
PROJECT LEADER: C. E. Thomas
PERIOD COVERED: November, 1989

I. PROJECT ART

A. Objective: Measure mainstream deliveries of gaseous ammonia by TDL and total ammonia by ion chromatography, and use the ratio of NH_3 to NH_4+ to calculate a value proportional to the basicity of ART cigarette smoke.

B. Results: The ammonia deliveries of ART cigarettes, when measured by both the TDL and the ion chromatography procedures, can be divided into gaseous ammonia (NH_3) and ammonium ion (NH_4+). A relative value of basicity of the smoke can be calculated using the ratio of NH_4+/NH_3 and the pK_a of ammonia. The table below shows the results of these calculations for a monitor #25, a production Merit ,and a production ART from the manufacturing Center.

Sample	Gaseous Ammonia (µg/cigt.)	Ammonium Ion (µg/cigt.)	Basicity (~pH)
MON #25	2.1	26.9	8.13
Merit 85	1.5	17.5	8.17
ART(X9FP)	4.0	26.0	8.43

C. Conclusions: The basicity of the smoke of ART production model as expressed in pH units was higher than both Merit and Monitor #25 Cigarettes. This result agrees with previous studies which have shown that ART cigarettes have higher deliveries of basic components such as pyridines and pyrazines in MS smoke condensate.

D. Plans: No further work in this area of investigation is planned. The project will however support requests for total ammonia in MS smoke.

E. References:

Parrish, M., Notebook #8858, p. 40.

II. MAINSTREAM AND SIDESTREAM SMOKE STUDIES

A. Objective: To develop a method for multicomponent quantitative analysis of the gaseous components of mainstream smoke using FT-IR spectroscopy.

B. Results: The deliveries of acetaldehyde, HCN, NO, and CO for a monitor #25 were measured using a newly developed method for gaseous components in MS smoke based on quantitation by FTIR spectroscopy. The measurements were made at a relatively low

spectral resolution of two wavenumbers to mimic the ability of low cost FTIR spectrometers to use the method. Absorption peaks for each gas were selected that varied linearly with concentration within the range found in cigarette smoke. A dilution factor of approximately 7 brought all four gases within the linear range. Sets of 5 monitor M25 cigarettes were smoked on two separate days. The deliveries of acetaldehyde, HCN, NO, and CO as measured by this method were 850±20 µg/cigt, 210±10 µg/cigt., 300±10 µg/cigt., and 15.5±5 mg/cigt. respectively. Except for the delivery of acetaldehyde these values are in excellent agreement with the gas phase deliveries as measured by reference methods. The concentration of acetaldehyde is approximately 15% high compared to values measured by dinitro-phenyhydrazone derivatization and HPLC analysis. This is due to interferences from other smoke aldehydes and ketones.

C. **Conclusions**: The FTIR analysis method for HCN, NO, and CO has been shown to be a suitable method of quantitation of these components in MS gas phase. However, further studies need to address the selection of spectral bands to more accurately quantify acetaldehyde.

D. **Plans**: To purchase a low cost FTIR and interface it with a five port smoking machine such as is used in CI. Possible improvements in the data analysis algorithms will be investigated. Programs will be written to automate the analysis procedure. The feasibility study results will be presented to Jane Lewis.

E. **References**:

Koller, K., PM Notebook 8870.

A. **Objective**: To develop methodology for studying SS odor and irritancy

B. **Results**: A sidestream collection chamber, designed by B. Jenkins, was positioned in line with a cambridge filter pad. This arrangement first entrained the whole smoke, then the pad removed the particulate phase of the smoke isolating the vapor phase components for further study. A gas phase fractionation system was interfaced to this collection system to collect the gas phase components for GC analysis. The fractionation system was designed based on the breakthrough phenomenon of polymeric adsorbents and cryogenic trapping. Glass tubes containing adsorbents of differing surface areas, Carbotrap C (12 m^2/g) and Carbosieve (550 m^2/g), were positioned after the Cambridge pad. At a given flow rate, compounds with higher volatility are subjected to less retention and therefore, exit from the adsorbent tube. By varying the amount of adsorbent, fractions containing compounds with different volatility were isolated. The gaseous stream exiting the system can be sampled via a heated gas sampling valve at different time intervals and injected into a gas chromatograph for

analysis via cryogenic focusing. At the exit port of the sampling valve, various fractions of the SS gas phase were evaluated for their odor properties. Those compounds retained by the adsorbents or cold traps were also evaluated.

C. **Conclusions**: The fractionation methods using either adsorbents or cold traps offer the flexibility to combine fractions to study the synergistic effects. With charcoal filters, the fractions which contained highly volatile compounds gave ammonia-like, fishy and pungent odor. Fractions with higher complexity, isolated by Carbotrap C , were very harsh and irritating in addition to the ammonia-like odor. Compounds retained by the Carbotrap had odors which were highly smoky and stale, similar to ashtray aroma.

D. **Plans**: Continue the fractionation experiments and establish the relationship of odor/irritancy versus volatility and functionality.